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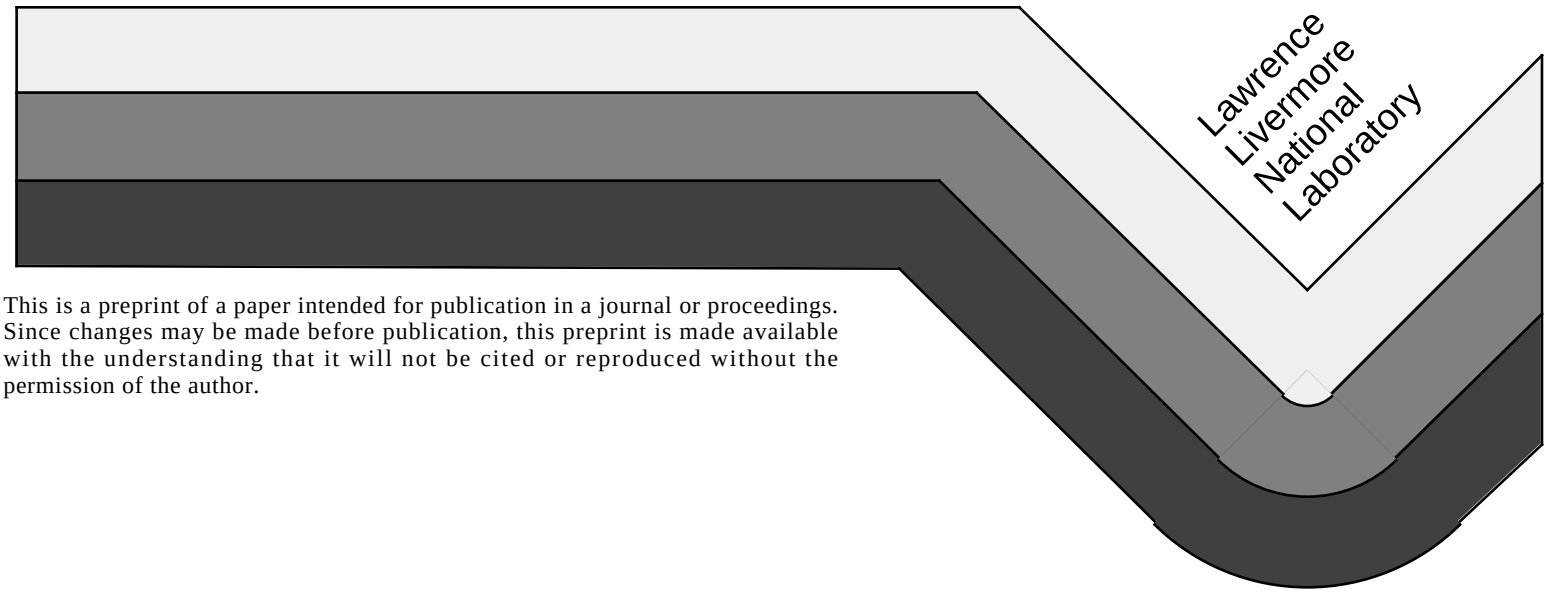

THE CONCENTRATION-ESTIMATION PROBLEM FOR MULTIPLE-WAVELENGTH DIFFERENTIAL ABSORPTION LIDAR

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Abstract. We are seeking to develop a reliable methodology for multi-chemical detection and discrimination based upon multi-wavelength differential absorption lidar measurements. In this paper, we summarize some preliminary results of our efforts to devise suitable concentration-estimation algorithms for use in detection and discrimination schemes.

Introduction

The utility of differential absorption lidar (DIAL) systems for remote, simultaneous sensing of multiple chemical species depends critically upon the ability to detect and estimate chemical concentrations in the presence of system uncertainty and measurement noise. We are seeking to develop a reliable methodology for the detection and discrimination of multiple chemicals based on DIAL measurements made at multiple wavelengths. In particular, we are interested in devising algorithms that can overcome the known deficiencies of simple signal averaging techniques used for two-wavelength DIAL[1-4] and can provide reliable estimates under the conditions of weak absorption, low signal-to-noise ratios, and correlated speckle noise.

In this paper, we summarize some preliminary results of our efforts to devise suitable concentration-estimation algorithms for use in detection and discrimination schemes. We pose the problem as a state-estimation problem. We establish conditions for state-observability, that is, conditions that concentrations are uniquely determined by a history of lidar return power measurements taken over a finite time-interval. We then present an estimator that is a simple generalization of the usual "log-ratio averaging" method for processing two-wavelength DIAL measurements. We discuss the properties of this estimator and identify its shortcomings. Finally, we summarize our efforts to develop a more general framework for solving the concentration-estimation problem based upon Kalman filtering theory.

Problem Statement

Consider the problem of estimating simultaneously the path-integrated concentrations of N chemicals using lidar measurements at M wavelengths, where $M > N$. The measured lidar return power p_i at wavelength i produced by backscatter from the atmosphere or a topological target at range r is

$$p_i(t) = E_T K(r) s_i(t) \exp\left\{-2\left(\sum_{j=1}^{N} \rho_{ij} y_j(t) + \alpha_i(r)\right)\right\} + n_i(t) \qquad i = 1, 2, \ldots, M \qquad (1)$$

where E_T is the transmitted energy, $K(r)$ is a range and system dependent parameter, $s_i(t)$ is the speckle modulation factor, ρ_{ij} is the absorptivity of chemical j at wavelength i, y_j is the path-integrated concentration of chemical j, α_i is the background extinction term, and n_i is receiver noise.

To apply equation (1) directly to estimate concentration requires a precise knowledge of parameters that are either unknown or known with only poor accuracy. To overcome this difficulty, the usual two-wavelength DIAL approach is to consider the logarithm of the ratio of the return powers.[3] In the M-wavelength generalization, we have a collection of M-1 "pseudo-measurements" of the form

$$z_i(t) = \frac{1}{2}\ln\left(\frac{p_{i+1}(t)}{p_i(t)}\right) \qquad i = 1, 2, \ldots, M\text{-}1 \tag{2}$$

The motivation for this approach is that, in the absence of measurement noise, Equation (2) reduces to

$$z_i = \sum_{j=1}^{N}\left(\rho_{ij} - \rho_{i+1,j}\right)y_j + \left(\alpha_i - \alpha_{i+1}\right) + \frac{1}{2}\ln\left(\frac{s_{i+1}}{s_i}\right) \tag{3}$$

which is linear in the unknown path-integrated concentrations and depends only on the differences in parameters. If we neglect the last two terms in (3) and set $M = 2$ and $N = 1$, we have the classical 2-wavelength, 1-chemical DIAL result:

$$y = \frac{\ln\left(p_2/p_1\right)}{2\left(\rho_1 - \rho_2\right)} \tag{4}$$

To complete the description of the problem, a model defining the temporal evolution of the path-integrated concentrations is required. It appears that most existing studies have assumed that the path-integrated concentrations are either time-invariant or can be modeled by a random walk process. However, a more general stochastic model may be necessary in many realistic applications.

The basic estimation problem of interest may then be posed as follows: *given* (i) a mathematical model describing the dynamic behavior of the path-integrated concentrations, (ii) models defining the speckle and receiver noise dynamics and statistics, and (iii) the measurement model defined by (1)-(2), *find* minimum error estimates of the path-integrated concentrations based on a knowledge of these models and a set of lidar measurements.

System Observability

An important aspect of any estimation problem is the existence of unique solutions. For the DIAL problem, the issue of interest is whether or not concentrations can be calculated uniquely by observing the vector of pseudo-measurements $\mathbf{z}(t)$ during some finite time-interval. In other words, it is important to rule out the situation in which two distinct concentration profiles give rise to identical measurement histories. From a system-theoretic viewpoint, this involves the notion of *state-observability*. For a system with state vector $\mathbf{x}$ and observation vector $\mathbf{z}$, we say that the state $\mathbf{x}(t')$ is *observable* over an interval $[t', T]$ if, and only if, it is uniquely determined by $\{\mathbf{z}(t): \; t' \le t \le T\}$ and the system is *completely observable* if every $\mathbf{x}(t')$ is observable. Complete observability is an important system requirement for the proper operation of any state-estimation algorithm.[5] Therefore, it is important that we establish the observability conditions for the multi-chemical, multi-wavelength DIAL problem before we begin to design and analyze estimation techniques for the problem.

As a first step in studying the observability problem, we assume that the vector of path-integrated concentrations $\mathbf{y}(t)$ is the output of a linear time-invariant process model of the form

$$\begin{aligned}\dot{\mathbf{x}}(t) &= \mathbf{A}\mathbf{x}(t) + \mathbf{w}(t)\\ \mathbf{y}(t) &= \mathbf{C}\mathbf{x}(t)\end{aligned} \tag{5}$$

where **x** is a state vector and **w** is a process noise vector. This model includes as special cases the two cases that have been commonly assumed in the DIAL literature, namely, the case when **y** is a constant and the case when **y** is the output of a random walk process. We also assume that the measurement model is defined by (1)-(2) and that the speckle modulation is a measurement noise, not a process state. Different observability conditions arise if speckle is modeled as a process state and these conditions are presently under investigation.

Observability conditions are then derived assuming that all inputs and noise terms in the system and measurement models are known. In this case, the process noise $\mathbf{w}(t)$ and measurement noise $\mathbf{n}(t)$ vanish and each element of the speckle modulation vector $\mathbf{s}(t)$ is unity. The measurement equation (2) then simplifies to

$$\mathbf{z}(t) = \mathbf{R}\mathbf{y}(t) + \varepsilon \tag{6}$$

where $\mathbf{R}$ is an $(M\text{-}1) \times N$ matrix and ε is an M-1 vector with entries defined by

$$r_{ij} = \rho_{ij} - \rho_{i+1,j} \tag{7}$$

and

$$\varepsilon_i = \alpha_i - \alpha_{i+1} \tag{8}$$

We can then easily establish observability conditions, which we now state without proof:

- The system defined by (5)-(6) is completely observable if, and only if, rank($\mathbf{O}$) = p, where

$$\mathbf{O} = \begin{bmatrix} \mathbf{RC} \\ \mathbf{RCA} \\ \vdots \\ \mathbf{RCA}^{p-1} \end{bmatrix} \tag{9}$$

and p is the dimension of the state **x**.

- If the system (5) is completely observable and rank($\mathbf{R}$) = N, then the system (5)-(6) is completely observable.
- If $\mathbf{y}(t)$ is a constant for all t, then it is observable if, and only if, rank($\mathbf{R}$) = N.

The first condition is the most general result and follows directly from well-known results of linear systems theory.[6] The second two results are corollaries of this condition. Note that observability imposes a requirement on **R** and, consequently, on the selection of the wavelengths employed in the DIAL system. Our results indicate that insuring observability should not be a major problem in practice.

Markov Estimator

We now present a simple estimator that is a generalization of the familiar 2-wavelength, 1-chemical DIAL result for the case of M wavelengths and N chemicals. This estimator is a generalized least squares estimator. It is also known as a *Markov estimator*. The estimator relies upon the following three assumptions: (i) $\mathbf{y}(t)$ is constant for all t, (ii) $\mathbf{y}(t)$ is observable (i.e., rank($\mathbf{R}$) = N), and (iii) the measurements satisfy

$$\mathbf{z}(t) = \mathbf{R}\mathbf{y} + \varepsilon + \mathbf{v}(t) \tag{10}$$

where the vector $\mathbf{v}(t)$ is zero-mean white noise with positive-definite covariance matrix Λ, that is,

$$E\{\mathbf{v}(t)\} = \mathbf{0} \tag{11}$$

$$E\{\mathbf{v}(t)\mathbf{v}(s)^T\} = \Lambda\delta(t-s) \tag{12}$$

Equation (10) is an approximation to (2) in which the contributions of speckle modulation and receiver noise are aggregated into the single variable $\mathbf{v}(t)$.

Now suppose that measurements are made at k time-instants $t_1, t_2, \ldots, t_k$. The Markov estimator based on these measurements is defined by

$$\hat{\mathbf{y}}_k = \text{argmin}_{\mathbf{y}}\left\{\sum_{i=1}^{k}\left(\mathbf{z}(t_i) - \mathbf{R}\mathbf{y} - \varepsilon\right)^T \Lambda^{-1}\left(\mathbf{z}(t_i) - \mathbf{R}\mathbf{y} - \varepsilon\right)\right\} \tag{13}$$

By carrying out the indicated minimization, it is a simple matter to show that the estimator is

$$\hat{\mathbf{y}}_k = \left(\mathbf{R}^T\Lambda^{-1}\mathbf{R}\right)^{-1}\mathbf{R}^T\Lambda^{-1}\left\{\frac{1}{k}\sum_{i=1}^{k}\mathbf{z}(t_i) - \varepsilon\right\} \tag{14}$$

Note that this estimator utilizes the sample average of k pseudo-measurements and represents the generalization of the usual "log-before-averaging" technique for 2-wavelength DIAL.[4] It is also clear that neglecting the extinction term ε, as is commonly done for 2-wavelength DIAL, will contribute a bias to the estimator.

The estimator defined by (14) possesses three important properties under the condition that (10)-(12) hold *exactly*. First, it is an unbiased, minimum variance estimator of $\mathbf{y}$. The covariance matrix is

$$\text{Cov}(\hat{\mathbf{y}}_k) = E\left\{\left(\hat{\mathbf{y}}_k - \mathbf{y}\right)\left(\hat{\mathbf{y}}_k - \mathbf{y}\right)^T\right\} = \frac{1}{k}\left(\mathbf{R}^T\Lambda^{-1}\mathbf{R}\right)^{-1} \tag{15}$$

which clearly demonstrates that the goodness of concentration estimates depends upon the absorption coefficients and hence on the particular choice of lidar wavelengths. (Note also that the assumption of observability insures that the inverse exists.) Second, the estimator is *consistent* in the sense that it converges to $\mathbf{y}$ in the mean-square sense as $k \to \infty$. Finally, if $\mathbf{v}(t)$ is also Gaussian, then the estimator is the maximum likelihood estimator based upon k measurements. In fact, it includes as a special case ($k = 1$) the single-sample maximum likelihood estimator derived by Warren[7] for multi-wavelength DIAL.

Unfortunately, Equations (10)-(12) cannot hold exactly, and thus these properties hold at best only approximately. In fact, it can be shown that the estimator is always biased and is neither minimum variance nor consistent, even when $\mathbf{s}(t)$ and $\mathbf{n}(t)$ are each white noise processes.

The Markov estimator also has two other shortcomings that seriously limit its usefulness in general DIAL applications. First, it assumes constant path-integrated concentrations. It provides, therefore, no means to account for temporal variations in the path-integrated concentrations that will invariably be present in most realistic applications of DIAL. Second, it is inadequate in its treatment of the noise sources. It does not distinguished between the receiver noise and speckle modulation effects, and thus it provides no simple way of identifying the relative contributions of these noise sources to the estimation error. Furthermore, the approach is not well-suited to problems with correlated speckle noise.

Kalman Filtering Approach

To accommodate both a more general dynamic model and a more rigorous treatment of system and measurement uncertainty than is permissible with the Markov estimator (or any other generalization of current signal averaging techniques for two-line DIAL), a more general estimation framework is required. We are presently looking to Kalman filtering theory to provide this framework.[5]

Several researchers have already recognized the potential application of Kalman filtering theory to DIAL problems.[8-10] However, little attention seems to have been given to establishing bias, efficiency, and convergence properties of filtering algorithms in this application. Moreover, it is unclear at present if a Kalman filtering approach will be effective under the conditions of primary interest to us, namely, under conditions of low absorptivity, high process model uncertainty, low signal-to-noise ratios, and correlated speckle noise. We are seeking to address these issues both analytically and computationally. We have developed codes for implementing Kalman filtering algorithms for both linear and nonlinear estimation problems and are beginning to apply them to the DIAL problem. We are also beginning to develop a capability for defining detailed system and measurement models to simulate multi-wavelength, multi-chemical problems and to provide synthetic data for testing our signal processing algorithms. Ultimately, we hope to have a computational tool that will permit us to design, analyze, and compare various signal averaging and estimation algorithms relative to one another and to establish performance bounds under various problem conditions.

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